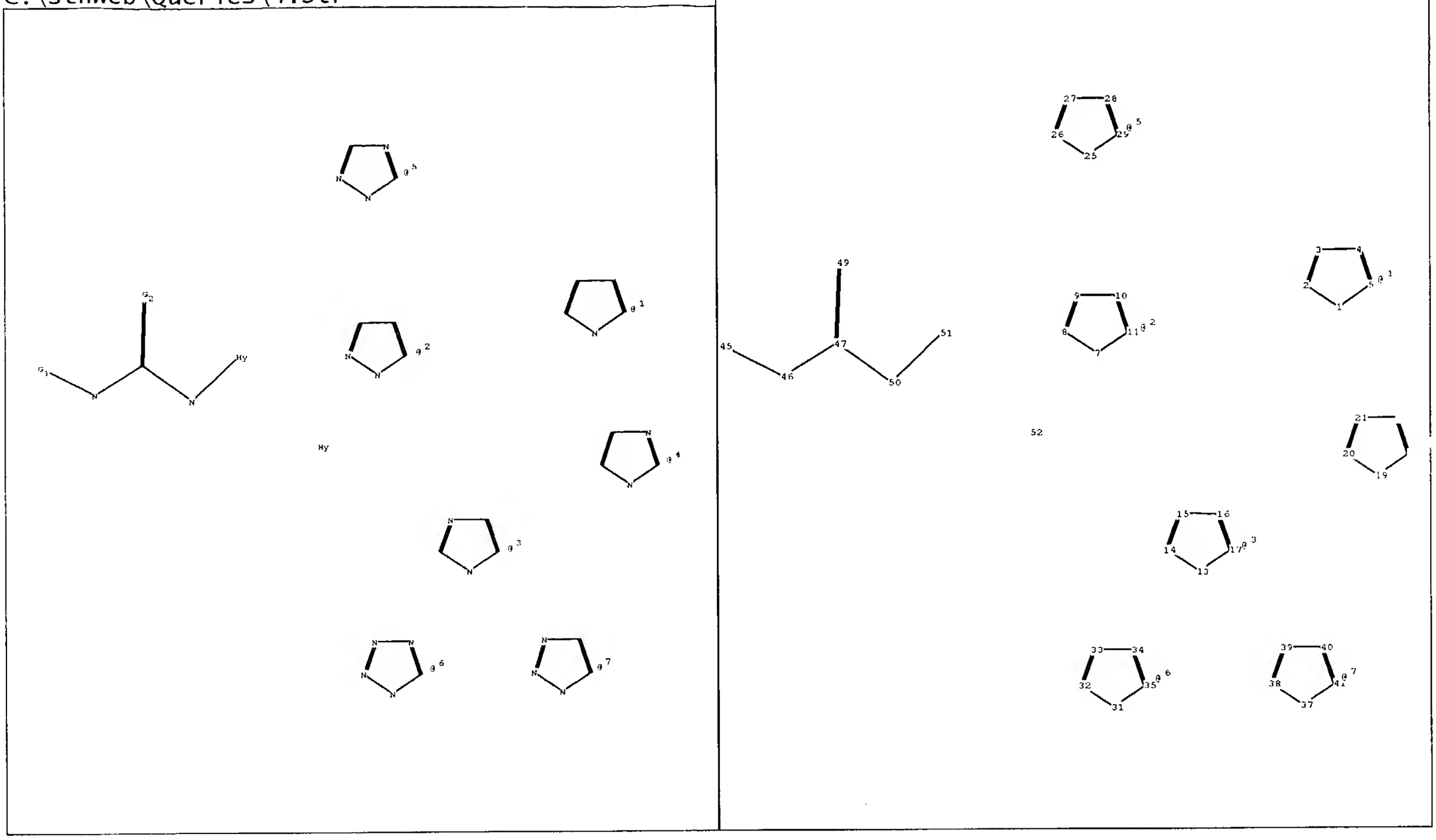
C:\stnweb\Queries\4.str



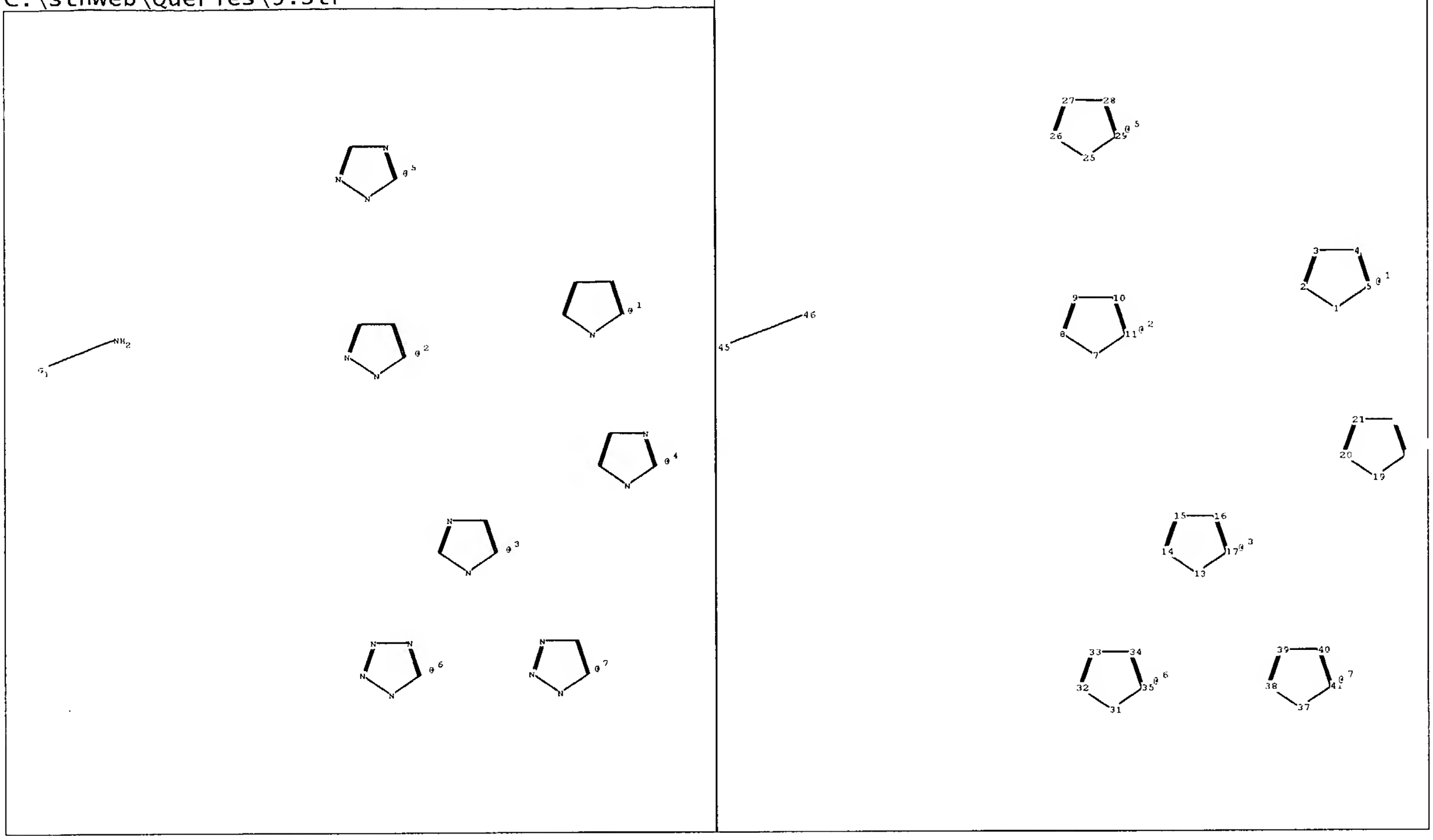

```
chain nodes :
    45  46  47  49  50  51  52
ring nodes :
    1  2  3  4  5  7  8  9  10  11  13  14  15  16  17  19  20  21  22  23  25  26  27  28
    29  31  32  33  34  35  37  38  39  40  41
chain bonds :
    45-46  46-47  47-49  47-50  50-51
ring bonds :
    1-2  1-5  2-3  3-4  4-5  7-8  7-11  8-9  9-10  10-11  13-14  13-17  14-15  15-16  16-17
    19-20  19-23  20-21  21-22  22-23  25-26  25-29  26-27  27-28  28-29  31-32  31-35  32-33
    33-34  34-35  37-38  37-41  38-39  39-40  40-41
exact/norm bonds :
    1-2  1-5  7-8  7-11  8-9  13-14  13-17  14-15  15-16  19-20  19-23  20-21  21-22  22-23
    25-26  25-29  26-27  27-28  28-29  31-32  31-35  32-33  33-34  34-35  37-38  37-41  38-39
    39-40  45-46  46-47  47-49  47-50  50-51
exact bonds :
    2-3  3-4  4-5  9-10  10-11  16-17  40-41
isolated ring systems :
    containing 1 : 7 : 13 : 25 : 31 : 37 :


G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

G2:O,S

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  7:Atom  8:Atom  9:Atom  10:CLASS  11:Atom
    13:Atom  14:Atom  15:Atom  16:Atom  17:Atom  19:Atom  20:Atom  21:Atom  22:Atom  23:Atom
    25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  31:Atom  32:Atom  33:Atom  34:Atom  35:Atom
    37:Atom  38:Atom  39:Atom  40:Atom  41:Atom  45:CLASS  46:CLASS  47:CLASS  49:CLASS
    50:CLASS  51:Atom  52:Atom
```

C:\stnweb\Queries\5.str

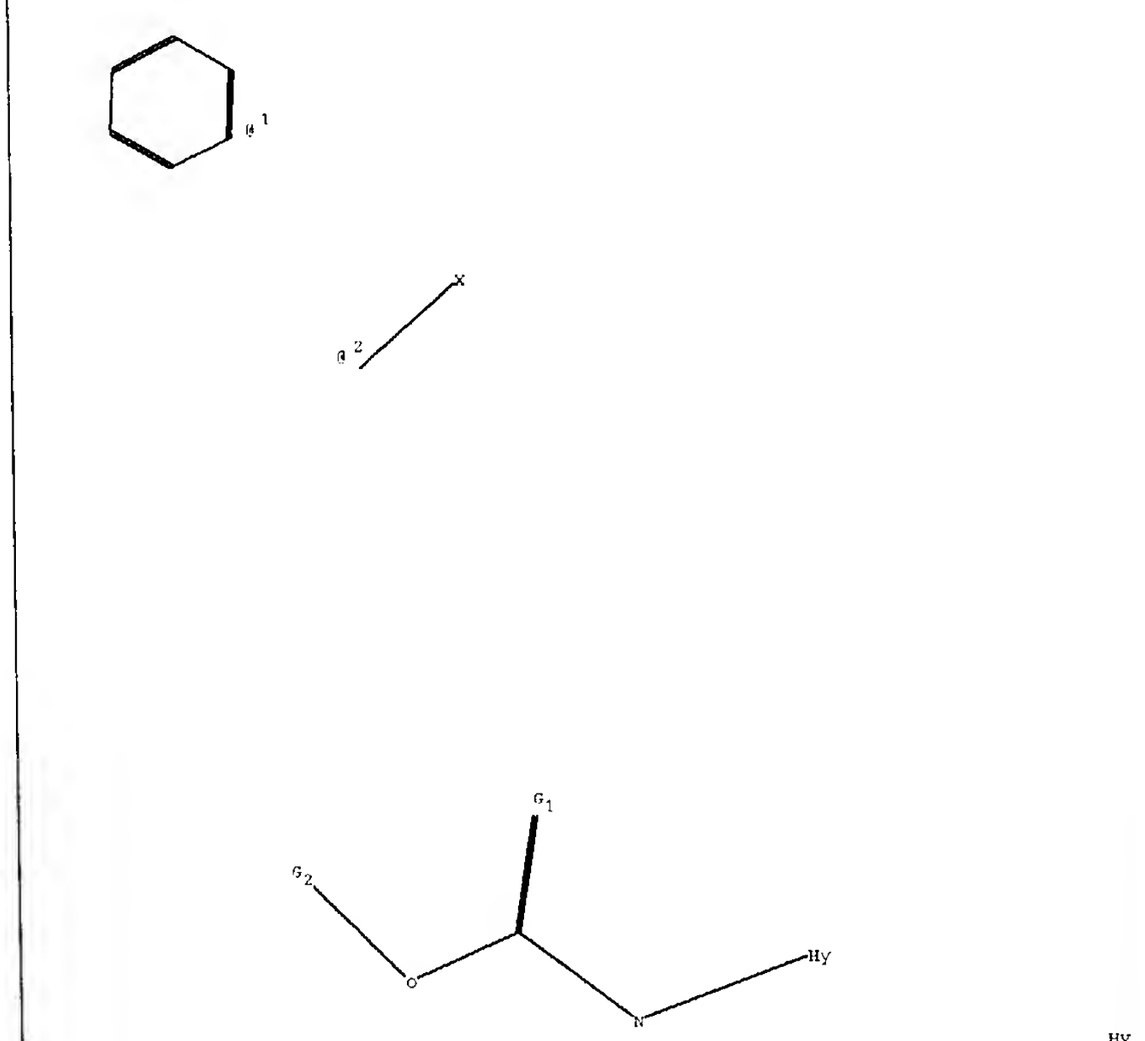


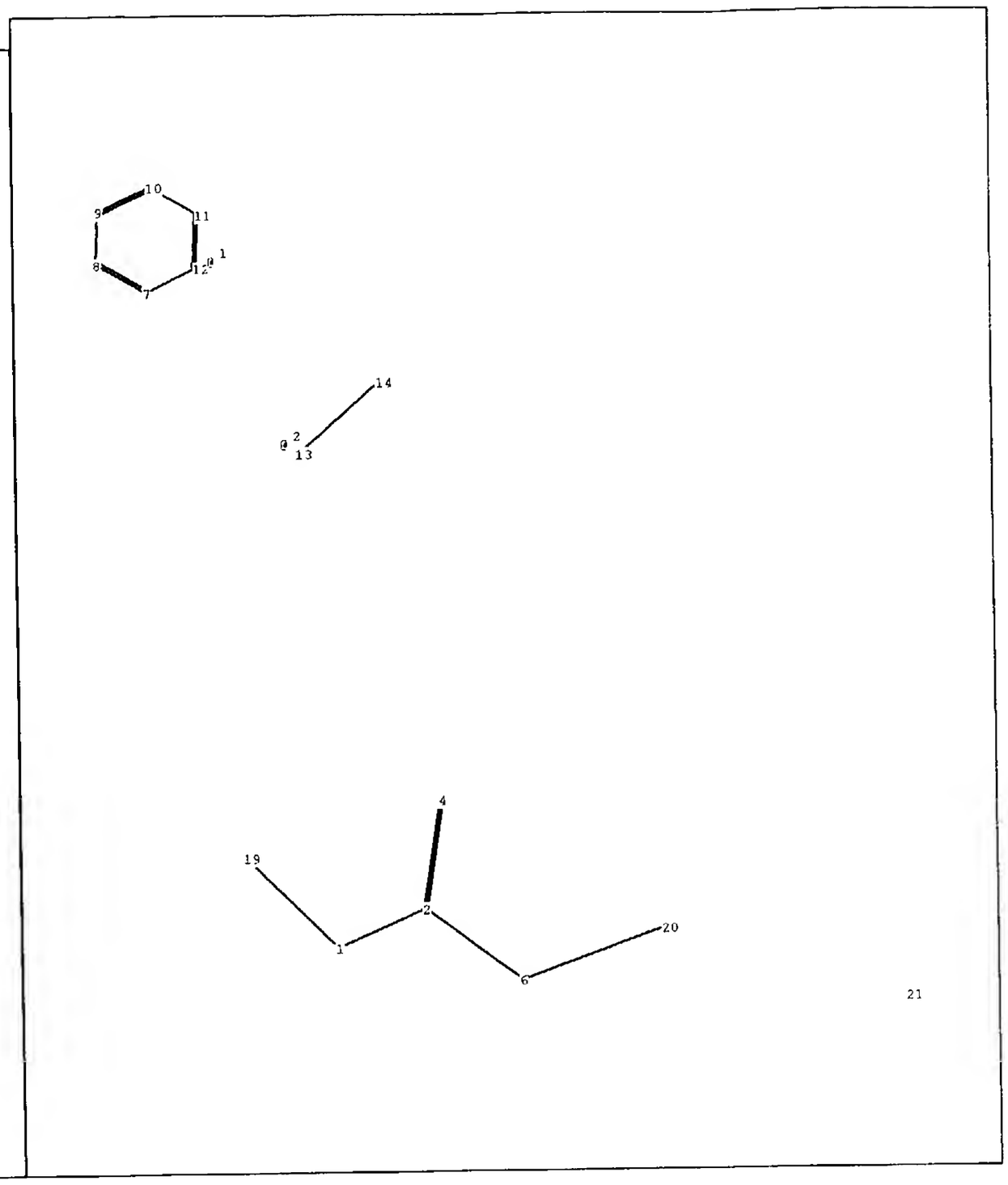
chain nodes :
45 46
ring nodes :
1 2 3 4 5 7 8 9 10 11 13 14 15 16 17 19 20 21 22 23 25 26 27 28
29 31 32 33 34 35 37 38 39 40 41
chain bonds :
45-46
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-8 7-11 8-9 9-10 10-11 13-14 13-17 14-15 15-16 16-17
19-20 19-23 20-21 21-22 22-23 25-26 25-29 26-27 27-28 28-29 31-32 31-35 32-33
33-34 34-35 37-38 37-41 38-39 39-40 40-41
exact/norm bonds :
1-2 1-5 7-8 7-11 8-9 13-14 13-17 14-15 15-16 19-20 19-23 20-21 21-22 22-23
25-26 25-29 26-27 27-28 28-29 31-32 31-35 32-33 33-34 34-35 37-38 37-41 38-39
39-40 45-46
exact bonds :
2-3 3-4 4-5 9-10 10-11 16-17 40-41
isolated ring systems :
containing 1 : 7 : 13 : 25 : 31 : 37 :

G1:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom
37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 45:CLASS 46:CLASS

C:\stnweb\Queries\5.str





chain nodes :
1 2 4 6 13 14 19 20 21
ring nodes :
7 8 9 10 11 12
chain bonds :
1-2 1-19 2-4 2-6 6-20 13-14
ring bonds :
7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-2 1-19 2-4 2-6 6-20
exact bonds :
13-14
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 7 :

G1:O,S

G2:[*1],[*2]

Match level :
1:CLASS 2:CLASS 4:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:CLASS 14:CLASS 19:CLASS 20:Atom 21:Atom

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 16:21:26 ON 18 JUN 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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DICTIONARY FILE UPDATES: 17 JUN 2004 HIGHEST RN 694921-36-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e isoquinoline/cn
E1              1      ISOQUINOLIN-7-YL TRIFLUOROMETHANESULFONATE/CN
E2              1      ISOQUINOLINAMINE, 1,3-DICHLORO-/CN
E3              1 --> ISOQUINOLINE/CN
E4              1      ISOQUINOLINE 1-(3-(BENZYLOXY)-4-METHOXYBENZYL)-3,4-DIHYDRO-6
                       -METHOXY-, PICRATE/CN
E5              1      ISOQUINOLINE 1-OXIDOREDUCTASE/CN
E6              1      ISOQUINOLINE 1-OXIDOREDUCTASE (ALPHA SUBUNIT) OXIDOREDUCTASE
                        PROTEIN (RALSTONIA SOLANACEARUM STRAIN GMI1000 GENE IORA2)/
                       CN
E7              1      ISOQUINOLINE 1-OXIDOREDUCTASE (CHROMOBACTERIUM VIOLACEUM STR
                       AIN ATCC 12472 GENE CV1674)/CN
E8              1      ISOQUINOLINE 1-OXIDOREDUCTASE (PSEUDOMONAS PUTIDA STRAIN KT2
                       440 GENE PP3947)/CN
E9              1      ISOQUINOLINE 1-OXIDOREDUCTASE (SHEWANELLA ONEIDENSIS STRAIN
                       MR-1 GENE SO3048 BETA SUBUNIT)/CN
E10             1      ISOQUINOLINE 1-OXIDOREDUCTASE (SHEWANELLA ONEIDENSIS STRAIN
                       MR-1 GENE SO3049 ALPHA SUBUNIT)/CN
E11             1      ISOQUINOLINE 1-OXIDOREDUCTASE, ALPHA SUBUNIT (CAULOBACTER CR
                       ESCENTUS GENE CC0022)/CN
E12             1      ISOQUINOLINE 1-OXIDOREDUCTASE, ALPHA SUBUNIT (CAULOBACTER CR
                       ESCENTUS GENE CC2270)/CN

=> s e3
L1              1 ISOQUINOLINE/CN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   119-65-3  REGISTRY
CN   Isoquinoline (6CI, 8CI, 9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   β-Quinoline
CN   2-Azanaphthalene
CN   2-Benzazine
CN   Benzopyridine
CN   Benzo[c]pyridine
CN   NSC 3395
FS   3D CONCORD
MF   C9 H7 N
CI   COM, RPS
LC   STN Files:   ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS,
       BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN,
       CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*,
       DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2,
       GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*,
       MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO,
       TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:   DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA  CAplus document type:  Book; Conference; Dissertation; Journal; Patent;
       Preprint; Report
```

```
RL.P      Roles from patents:  ANST (Analytical study); BIOL (Biological study);
          MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP
          (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in
          record)
RLD.P     Roles for non-specific derivatives from patents:  ANST (Analytical
          study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation);
          PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES
          (Uses)
RL.NP     Roles from non-patents:  ANST (Analytical study); BIOL (Biological
          study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
          (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
          (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP    Roles for non-specific derivatives from non-patents:  ANST (Analytical
          study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC
          (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);
          PRP (Properties); RACT (Reactant or reagent); USES (Uses)
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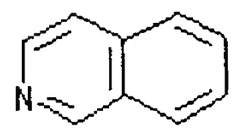

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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

             4006 REFERENCES IN FILE CA (1907 TO DATE)
              366 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
             4012 REFERENCES IN FILE CAPLUS (1907 TO DATE)
                9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)


=>
L2       STRUCTURE UPLOADED

=> d l2
L2 HAS NO ANSWERS
L2                STR

=> s l2
SAMPLE SEARCH INITIATED 16:34:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     661 TO ITERATE

100.0% PROCESSED      661 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:   ONLINE   **COMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:         11678 TO     14762
PROJECTED ANSWERS:                2 TO       124

L3             2 SEA SSS SAM L2

=> s l2 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:34:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  13265 TO ITERATE

100.0% PROCESSED   13265 ITERATIONS                                 43 ANSWERS
SEARCH TIME: 00.00.01
```

```
L4              43 SEA SSS FUL L2

=> file hcaplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       170.44     170.65

FILE 'HCAPLUS' ENTERED AT 16:34:43 ON 18 JUN 2004
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FILE COVERS 1907 - 18 Jun 2004  VOL 140 ISS 26
FILE LAST UPDATED: 17 Jun 2004  (20040617/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l4/prep
            15 L4
       3160985 PREP/RL
L5           13 L4/PREP
                  (L4 (L) PREP/RL)

=> s l5 and tan, Z?/au
          1084 TAN, Z?/AU
L6           0 L5 AND TAN, Z?/AU

=> s l5 and song, j?/au
          4830 SONG, J?/AU
L7           0 L5 AND SONG, J?/AU

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         7.08     177.73

FILE 'REGISTRY' ENTERED AT 16:36:37 ON 18 JUN 2004
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STRUCTURE FILE UPDATES:   17 JUN 2004  HIGHEST RN 694921-36-3
DICTIONARY FILE UPDATES:  17 JUN 2004  HIGHEST RN 694921-36-3
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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L8 STRUCTURE UPLOADED

=> d l8
L8 HAS NO ANSWERS
L8 STR

=> s l8
SAMPLE SEARCH INITIATED 16:38:06 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 24419 TO ITERATE

4.1% PROCESSED 1000 ITERATIONS 49 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

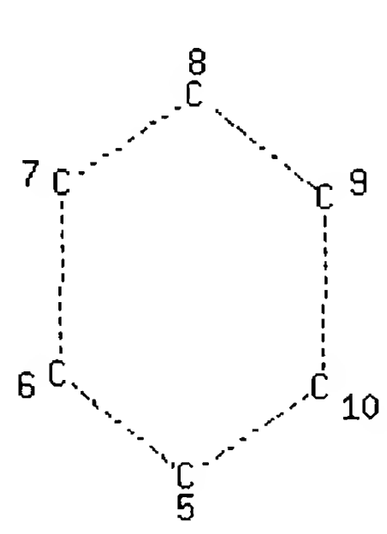
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 479039 TO 497721
PROJECTED ANSWERS: 21855 TO 26005

L9 49 SEA SSS SAM L8

=>
L10 STRUCTURE UPLOADED

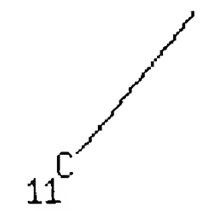
=> d l10
L10 HAS NO ANSWERS
L10 STR

0 16 S 17



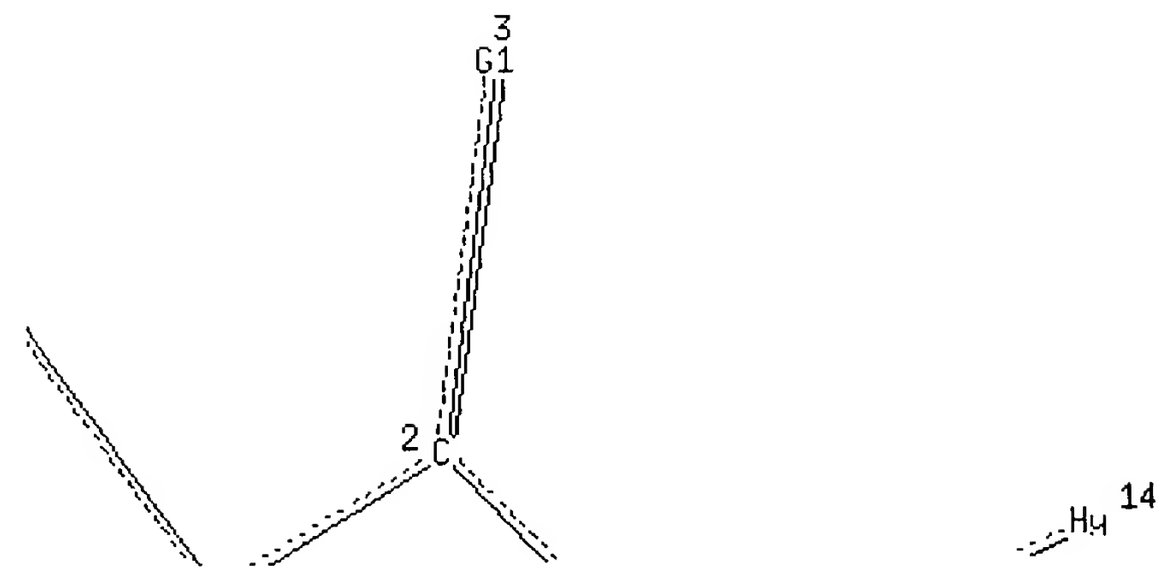
Page 1-A

Page 1-B

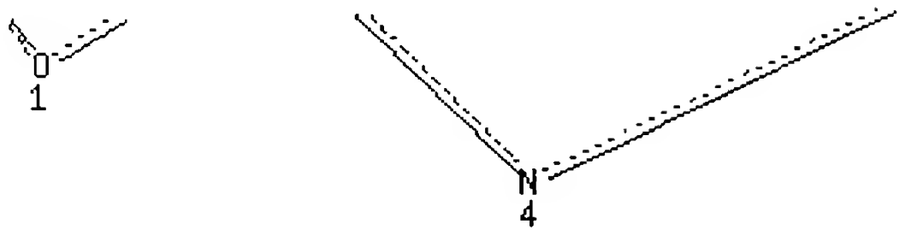


Page 2-B

Page 3-A



Page 3-B



Page 4-B

Hy 15

Page 4-C

VAR G1=16/17
VAR G2=10/11
NODE ATTRIBUTES:

NSPEC	IS C	AT	1
NSPEC	IS C	AT	2
NSPEC	IS C	AT	3
NSPEC	IS C	AT	4
NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS R	AT	7
NSPEC	IS R	AT	8
NSPEC	IS R	AT	9
NSPEC	IS R	AT	10
NSPEC	IS C	AT	11
NSPEC	IS C	AT	12
NSPEC	IS C	AT	13
NSPEC	IS C	AT	14
NSPEC	IS C	AT	15

DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 1 2 4 11 12 16 17
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I

```
NUMBER OF NODES IS  17

STEREO ATTRIBUTES: NONE


=> s l10
SAMPLE SEARCH INITIATED 16:41:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3872 TO ITERATE

 25.8% PROCESSED    1000 ITERATIONS                                 8 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:        73709 TO     81171
PROJECTED ANSWERS:             286 TO       952

L11             8 SEA SSS SAM L10

=> s l10 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 16:41:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  77434 TO ITERATE

100.0% PROCESSED   77434 ITERATIONS                               387 ANSWERS
SEARCH TIME: 00.00.02

L12           387 SEA SSS FUL L10

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             158.36     336.09

FILE 'HCAPLUS' ENTERED AT 16:41:29 ON 18 JUN 2004
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FILE COVERS 1907 - 18 Jun 2004  VOL 140 ISS 26
FILE LAST UPDATED: 17 Jun 2004  (20040617/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l12/rct
```

```
          222 L12
      2631689 RCT/RL
L13         69 L12/RCT
                (L12 (L) RCT/RL)

=> d his

     (FILE 'HOME' ENTERED AT 16:21:26 ON 18 JUN 2004)

     FILE 'REGISTRY' ENTERED AT 16:21:32 ON 18 JUN 2004
                E ISOQUINOLINE/CN
L1            1 S E3
L2              STRUCTURE UPLOADED
L3            2 S L2
L4           43 S L2 FULL

     FILE 'HCAPLUS' ENTERED AT 16:34:43 ON 18 JUN 2004
L5           13 S L4/PREP
L6            0 S L5 AND TAN, Z?/AU
L7            0 S L5 AND SONG, J?/AU

    FILE 'REGISTRY' ENTERED AT 16:36:37 ON 18 JUN 2004
L8              STRUCTURE UPLOADED
L9           49 S L8
L10             STRUCTURE UPLOADED
L11           8 S L10
L12         387 S L10 FULL

    FILE 'HCAPLUS' ENTERED AT 16:41:29 ON 18 JUN 2004
L13          69 S L12/RCT

=> s l13 and l5
L14           0 L13 AND L5

=> file caold
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                              ENTRY     SESSION
                                               2.36      338.45

FULL ESTIMATED COST

FILE 'CAOLD' ENTERED AT 16:41:59 ON 18 JUN 2004
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  This file supports REG1stRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

=> d his
```

```
      (FILE 'HOME' ENTERED AT 16:21:26 ON 18 JUN 2004)

      FILE 'REGISTRY' ENTERED AT 16:21:32 ON 18 JUN 2004
                E ISOQUINOLINE/CN
L1              1 S E3
L2                STRUCTURE UPLOADED
L3              2 S L2
L4             43 S L2 FULL

      FILE 'HCAPLUS' ENTERED AT 16:34:43 ON 18 JUN 2004
L5             13 S L4/PREP
L6              0 S L5 AND TAN, Z?/AU
L7              0 S L5 AND SONG, J?/AU

      FILE 'REGISTRY' ENTERED AT 16:36:37 ON 18 JUN 2004
L8                STRUCTURE UPLOADED
L9             49 S L8
L10               STRUCTURE UPLOADED
L11             8 S L10
L12           387 S L10 FULL

      FILE 'HCAPLUS' ENTERED AT 16:41:29 ON 18 JUN 2004
L13            69 S L12/RCT
L14             0 S L13 AND L5

      FILE 'CAOLD' ENTERED AT 16:41:59 ON 18 JUN 2004

=> s l4 and l12
                0 L4
                6 L12
L15             0 L4 AND L12

=>
```